5-«beta»-Cholestane, 3-«alpha»,7-«alpha»,12-«alpha»,27-tetraol, TMS

Other names: 5«beta»-Cholestane-3«alpha»,7«alpha»,12«alpha»,26-tetrol, TMS
Inchi: InChI=1S/C39H80O4Si4/c1-28(27-40-44(5,6)7)18-17-19-29(2)32-20-21-33-37-34(26-36(
InchiKey: FQRGIGVECJSGDA-RMFUMDPWSA-N
Formula: C39H80O4Si4
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(
Mol. weight [g/mol]: 725.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	11.819		Crippen Method
rinpol	3502.00		NIST Webbook
rinpol	3450.00		NIST Webbook
rinpol	3502.00		NIST Webbook
rinpol	3450.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R271684&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.